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Assessing the Environmental-Hazard Potential for Life Cycle Assessment, Eco-Efficiency and SEEbalance®

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Abstract**DOI:** <http://dx.doi.org/10.1065/lca2005.08.220>

Intention, Goal, Scope, Background. BASF has developed the eco-efficiency analysis tool to address not only strategic issues but also issues posed by the marketplace, politics and research. The goal was to develop a tool for supporting decision-making processes, which is useful for many of applications in the Chemical and other industries. A part of the eco-efficiency analysis involves the evaluation of the toxicity and the ecotoxicity potential.

Objectives. Many life cycle analyses do not include an assessment of the toxicity potential nor the ecotoxicity potential. However, in order to arrive at a comprehensive assessment of products and processes, it is often the ecotoxicity potential, which constitutes an important factor with regard to the evaluation of sustainability. The cradle-to-grave approach is also important for this calculation and will be done based on a database that will be discussed also in this paper.

Methods. The method used for the determination of the ecotoxicity potential follows the basic rules of the European Union Risk Ranking System (EURAM). The other criteria of the ecological fingerprint are combined with the economical results in the eco-efficiency portfolio.

Results and Discussion. The results of the studies are shown in a simple diagram, the eco-efficiency portfolio. Therefore ecological data are summarized in a special manner as described previously. It has been shown that the weighting factors, which are used in our method, have a negligible impact on the results. In most cases, the input data have the dominant impact on the results of the study. The ecotoxicity assessment will be a part of the ecological calculation. Because of the cradle-to-grave approach, substances of the whole life cycle can be identified that might have a toxic impact to the environment. The results can be used for optimization of the process.

Conclusions. The new calculation model allows the assessment of eco-toxicological substances in an appropriate and easy way. In most of the cases the data from a European safety data sheet are sufficient for the calculation. The normalized data can be incorporated very easily in the ecological fingerprint and in the drawing of the eco-efficiency portfolio.

Recommendations and Outlook. LCA in combination with the evaluation of the ecotoxicity potential will for reasons of optimizing for least impact become more important in certain cases. Especially in those systems where water emissions are likely, the use of the evaluation system in the eco-efficiency analysis is recommended. This new methodology allows the calculation of ecotoxicity potentials in a short time with a small set of input information. The analytical eco-efficiency tool helps in implementing more sustainable processes and products in the future.

Keywords: Eco-efficiency; eco-efficiency portfolio; ecology fingerprint; ecotoxicity assessment; metrics and measurement; sustainable development

Introduction

The quest for sustainable products and projects is gaining importance for industry. The economic success of companies depends increasingly on the extent to which they can meet the demands of sustainable development.

The World Business Council for Sustainable Development (WBCSD) defined eco-efficiency as a management philosophy in 1993 following the 1992 Rio Summit. Business was to be encouraged to become more competitive and innovative while at the same time exercising greater responsibility for the environment [1].

Eco-efficiency has been variously defined and analytically implemented by several workers. In most cases, eco-efficiency is taken to mean the ecological optimization of overall systems while not disregarding economic factors [2].

That is precisely why BASF has developed the eco-efficiency analysis, to enable early recognition and systematic detection of economic and environmental opportunities and risks in existing and future business activities. The description of the basic idea and of the details of the method was published with the example of dyeing Denim for jeans with Indigo [3,4]. At that time the ecological fingerprint included five categories; today it is expanded by the category 'land use'. A part of the ecological fingerprint was the assessment of the toxicity potential with a defined method also developed by BASF [5]. That was the starting point for gaining experience assessing ecotoxicity data. It was not possible to use R-phrases in the same manner as in the evaluation of human toxicity because of the need for additional information. Therefore a new system was developed for the calculation of the ecotoxicity potential as part of the BASF eco-efficiency analysis. This article will explain how the system works and how it can be incorporated in the eco-efficiency analysis as well as in the SEEbalance®, the sustainability analysis of BASF.

1 Life Cycle Assessment, Eco-Efficiency Analysis

The BASF eco-efficiency analysis is a tool for quantifying sustainability of products and processes. It provides an assessment of the total costs and environmental impact that a product or process creates over its complete life cycle, starting with raw material extraction and continuing on to post-

use disposal or recycling. The analysis includes an in-depth comparison of the pros and cons of various product alternatives, all of which fulfill the same customer need. Also included in the analysis is an examination of potential scenarios to check future developments and to assess uncertainties. Eco-efficiency analyses are useful for a sustainability analysis including consideration of social aspects.

- Supporting strategic decision-making
- Marketing: communicating with external customers
- Prioritizing R & D activities

Ecological data are calculated in accordance to the Life Cycle Assessment (LCA)-rules of ISO 14040ff as a first step. The data are then summarized into six main factors using a special method developed by BASF. Those six categories are considered in determining the environmental impact. They are: consumption of raw materials; energy consumption; emissions to the air, water and soil (wastes); toxicity potential of substances employed and produced, the risk potential of misuse; and the use of area. These parameters are weighted and combined to give an overall impact score. The six impact categories result is shown in an ecological fingerprint (Fig. 1).

The economic aspects of the alternative products or processes are represented in an overall cost calculation, taking into account the flow of material and energy and including all relevant secondary processes. Factors, which increase costs and potentials for cost reduction, are easily identified in the process.

Using the data on the relative cost and environmental impact, an eco-efficiency portfolio is created. This portfolio makes it easy to identify the strengths and weaknesses of a particular product.

The value of the eco-efficiency tool, apart from its description of the current state, lies in the recognition of important factors and in the illustration of 'what if ...?' scenarios.

The SEEbalance®, an instrument that includes an assessment of a product's social impacts in addition to the economic and environmental ones, is currently being developed [6].

2 Goal Setting

For a complete evaluation of substances, products and processes, together with the human toxicity, ecological aspects also need to be considered. A systematic evaluation of potential risks for man and environment caused by new and existing chemicals was started 1993 in the EU organization, which worked out Technical Guidance Documents (TGD) [7] for carrying out comprehensive risk assessments. Using those principles a method was developed that enables the calculation of ecological data within an LCA project. Analogous to the human toxicity model that was developed by BASF for using it in LCA and eco-efficiency calculations, the goal of creating a method for eco-toxicological data was set. While on one hand ecotoxicity potentials need to be calculated and assessed and on the other hand eco-efficiency studies have to be completed within a relatively short time, the evaluation of eco-toxicological effects for LCA must be done in a different, more simplified way than for a complete and comprehensive risk assessment. Moreover, data from a risk assessment are often not easily available or are too detailed for the use in the BASF tool. With regard to ecotoxicity various methods for the estimation of substances are available. In TGD a huge amount of different QSAR-methods are described. An overview of different QSAR models is given in [8]. However it is recommended that an experienced scientist should review the results of such estimation. So it was necessary to use easily accessible and sufficiently detailed data for all the products in the life cycle. They should reflect the properties of substances with reliable data, which can be used by everyone in industry and business. There should be a consistent algorithm to get results of ecotoxicity potentials always in a reproducible manner. The results must be transformed into a format, which can be incorporated into the eco-efficiency analysis spreadsheet to calculate the ecotoxicity potential as an environmental criterion. The excellent experiences we have had with the use of the human toxicity model showed the need for and support offered by such a calculation system in working out an eco-efficiency analysis or a SEEbalance.

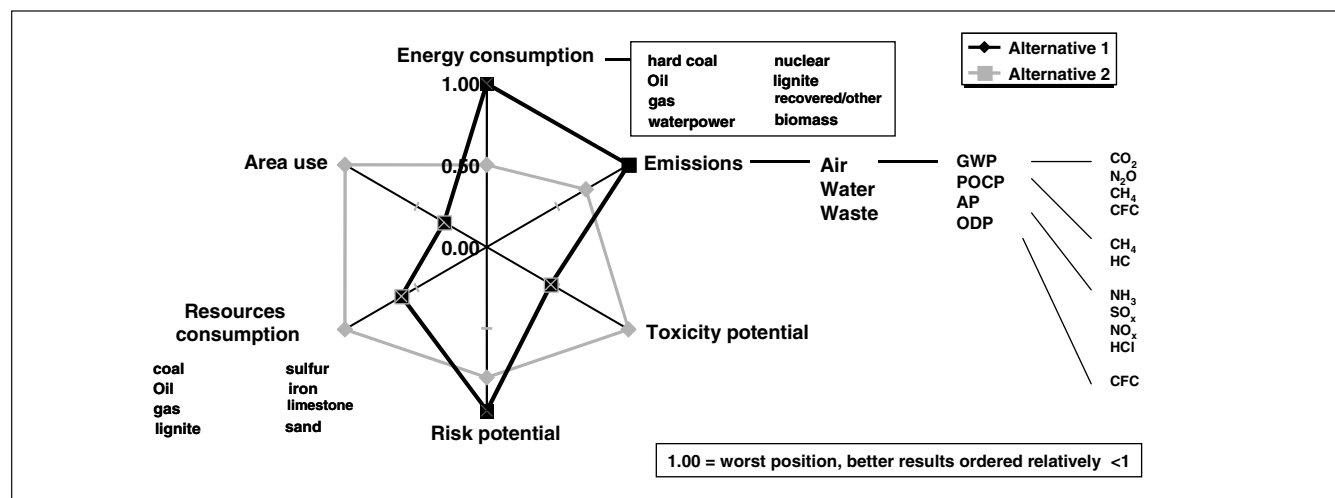


Fig. 1: The ecological fingerprint and the different categories behind the main factors

3 Ecotoxicity Assessments with a Scoring System

3.1 Basic assumptions

The ecological risk potential (P) of a substance is thought to be caused by (i) the environmental exposure (E) and (ii) its hazardous effects (H). This means the total ecological risk potential will be higher for score effects for prolonged exposures (Eq. 1).

Eq. 1: The calculation of the ecological risk potential (P)

$$P = E \times H$$

To compare substances with respect to their ecological risk potential a scoring system has been developed, based on European Union Risk Ranking System (EURAM) [8].

The environmental compartment selected for assessing ecotoxicological potential is the water. The reason for this choice

is that this compartment is often the most relevant one and most of the eco-toxicological data are available for aquatic organisms. Moreover, eco-toxicological data on aquatic species are used as basis for the classification and labeling of substances with respect to the environment.

The scoring system uses as factors the potential relevance for the aquatic environment (which we call potential environmental impact), the aquatic toxicity and the potential of bioaccumulation.

An overview of input data, factors and procedures for the derivation of the Environmental Score is given in Fig. 2. This Environmental score is derived from intrinsic properties of substances and therefore will result in a characteristic attribute that can be used to compare substances with respect to their potential to impact the environment. It will be used in defined steps of the evaluation of products in the eco-efficiency analysis.

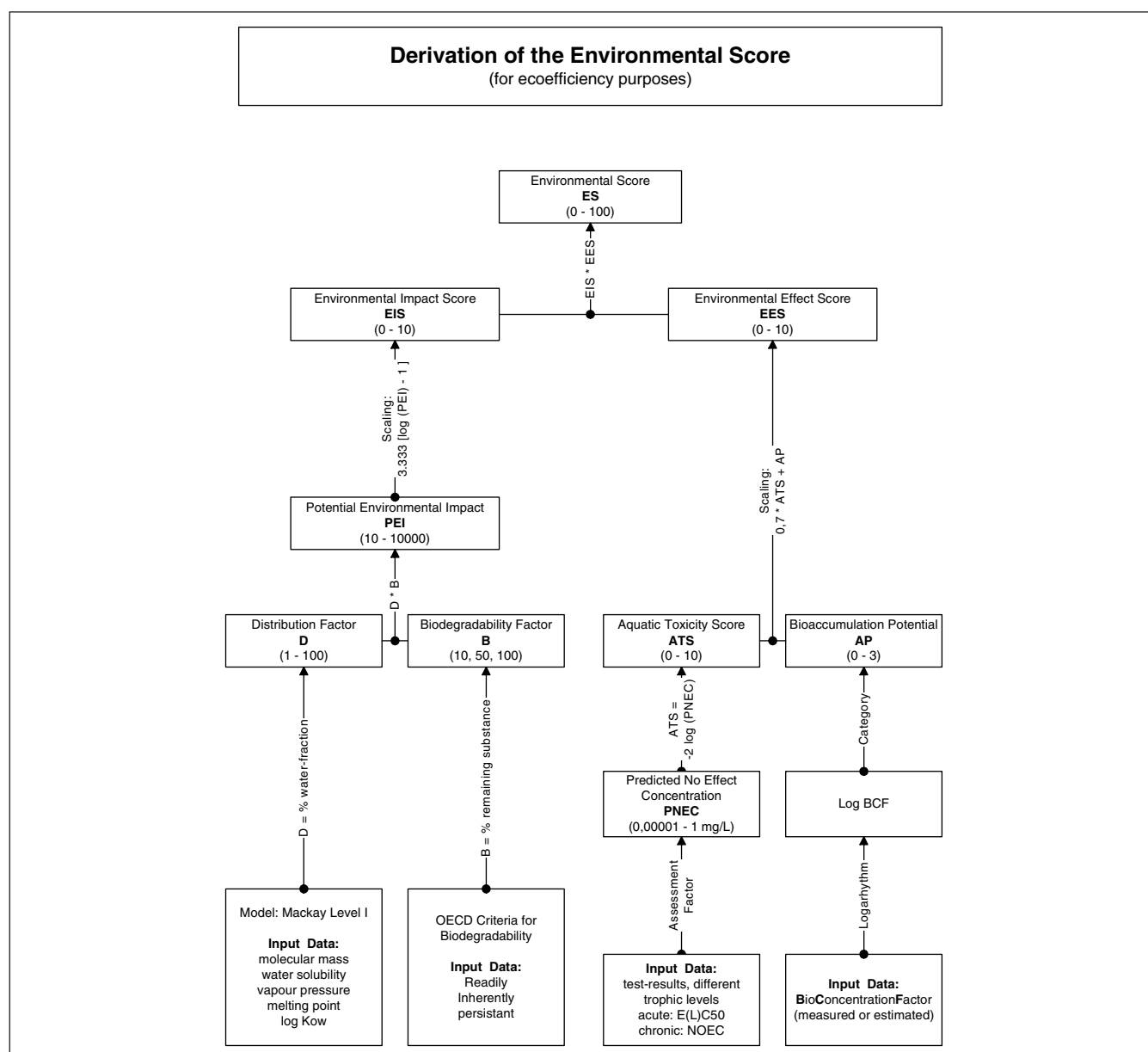
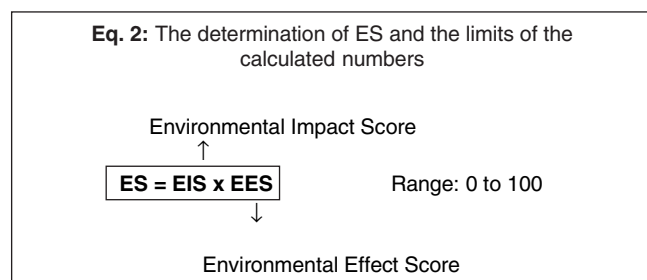


Fig. 2: Overview of the calculation of the Environmental Score ES

The system ranks substances taking into account their intrinsic properties (like physico-chemical and eco-toxicological data) and their fate in the environment. Although largely simplified, concepts and procedures of the environmental risk assessment are implemented in the method. It has to be noticed that the system is only suitable for comparing substances and that the risk or concern associated with a calculated score is only a potential, due to the fact that the emission of the substances into the environment during use is not considered in the model. The concentrations of the substances are calculated in the eco-efficiency analysis and are linked with the data from the Environmental score of the substances to the Environmental Hazard Potential. In this potential, substances over the whole life cycle are considered.

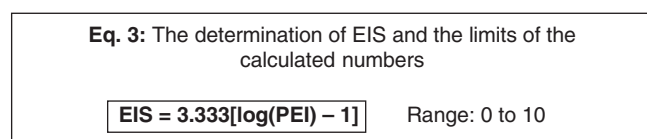
3.2 Environmental Score (ES)

The Environmental score (ES) is the product of the Environmental Impact Score (EIS) and Environmental Effect Score (EES) (Eq. 2):



3.3 Environmental Impact Score (EIS)

The logarithm of the Potential Environment Impact (PEI) is scaled to take values between 1 and 10 to obtain the Environmental Impact Score (EIS) (Eq. 3).



3.4 Potential Environmental Impact (PEI)

The combination of the Biodegradability Factor (B), expressed as the fraction remaining in the water, and the Distribution Factor (D) will end in the Potential Environmental Impact (PEI). It can be considered as a mass for the environmental exposure to a certain substance (Eq. 4).

Eq. 4: The determination of PEI and the limits of the calculated numbers

$$\text{PEI (Potential Environmental Impact)} = \text{Distribution (D)} \times \text{Biodegradation (B);}$$

Range: 10 to 10,000

3.4.1 Distribution in the aqueous system

For the calculation of the Potential Environmental Impact (PEI) it is necessary to establish the relevance of the aquatic compartment for the substance to be assessed. The Distribution Factor (D) is expressed as the percent fraction of the substance in the aquatic environment calculated with the multimedia model. It can vary between 1 and 100. In the case the calculated percentage remaining in water is <1, the fraction is set to one as default value.

The fraction in the aqueous compartment can be estimated by using a multimedia model of type Mackay level I [9] and with a few physico-chemical data of the compound taken from the Safety Data Sheet (MSDS) or from other sources in the literature. The physico-chemical properties needed to run the model are molecular mass (g/mol), water solubility (g/m³), vapour pressure (Pa), log K_{ow} and melting point (°C). The characteristics of the 'evaluative' environment and the software used for the calculation are available on the Internet [10].

3.4.2 The implementation of the biodegradability

Another important aspect to be considered for the calculation of the Potential Environmental Impact (PEI) is the determination of the potential for a substance to be biodegraded in the aquatic compartment. Biodegradation is indeed generally considered to be the main pathway for removal of chemicals from the environment; a rapidly biodegradable substance is therefore not expected to pose long-term risks for the environment.

The results of biodegradation tests conducted according to OECD Guidelines (and available for many substances) can be used to classify substances into different groups of biodegradability. Depending on the category of biodegradation the percentage of the substance remaining in the water is called the Biodegradability Factor (B) and is established according to **Table 1**.

If no experimental data are available the classification of a substance into a biodegradation class may be done using available estimating methods and the appropriate guidance to the interpretation of their results [11,12].

Table 1: Different groups of biodegradability of substances

Biodegradability (according to OECD criteria)	% Degraded	% Remaining	Factor B
Readily biodegradable	90	10	10
Inherently biodegradable	50	50	50
Persistent	0	100	100
Default	0	100	100

For substances for which no data on biodegradation are available and the results of estimates are considered unreliable, the default value -persistent- will be used.

3.5 Environmental Effect Score (EES)

The Environmental Effect Score (EES) is calculated combining the Aquatic Toxicity Score (ATS) and the potential for bioaccumulation (AP) of a substance. Eq. 5 leads to the calculation of the Environmental Effect Score (EES).

Eq. 5: The determination of EES and the limits of the calculated numbers

$$\text{EES} = 0.7 \times \text{ATS} + \text{AP} \quad \text{Range: 0 to 10}$$

Although the aquatic toxicity plays the major role in the determination of the environmental effect score, Eq. 5 enables bio-accumulative substances to get a significant score even if they are not particularly toxic to aquatic organisms.

3.6 Aquatic Toxicity Score (ATS)

The Aquatic Toxicity Score (ATS) is determined using the results of either acute or chronic toxicity studies on aquatic organisms (generally fish, daphnia and algae). If both chronic and acute tests are available for a substance, the acute tests are ignored. The lowest effect concentration expressed as L(E)C 50 or NOEC is selected and divided by an Assessment Factor (AF) to derive a PNEC (Predicted No Effect Concentration).

The assessment factor depends on the nature of the available test (chronic or acute endpoint) and on the number of the species tested. The selection of the appropriate assessment factor is made according to Table 2 and Eq. 6.

Eq. 6: The determination of PNEC

$$\begin{aligned} \text{PNEC} &= \text{NOEC} / \text{AF} \quad (\text{in the case chronic tests are available}) \\ \text{PNEC} &= \text{L(E)C 50} / \text{AF} \quad (\text{in the case only acute tests are available}) \end{aligned}$$

The Aquatic Toxicity Score (ATS) is then obtained according to Eq. 7.

Eq. 7: The determination of ATS and the limits of the calculated numbers

$$\text{ATS} = -2 \log(\text{PNEC}) \quad \begin{array}{l} \text{Range:} \quad 10 \text{ to } 0 \\ \text{Corresponds to: } 0.00001 \text{ mg/l} < \text{PNEC} < 1 \text{ mg/l} \end{array}$$

3.7 The potential for bioaccumulation in the assessment system (AP)

Bioaccumulation is defined as the tendency of a substance to accumulate in an organism from the surrounding environment. Together with the aquatic toxicity the potential for bioaccumulation plays a relevant role in the assessment of substances.

On the one hand through bioaccumulation the overall persistence of a substance is increased, on the other hand certain organisms can be indirectly exposed to bio accumulative substances via the food chain. Finally accumulated substances - may be remobilized in the organism (for example during the reproduction) and therefore exert toxic effect even if a direct exposure in the environment does not occur any longer.

As a measure for the potential for bioaccumulation the Bioconcentration Factor (BCF) is normally used. Experimentally derived BCFs are available only for few substances but they can be estimated using the partitioning coefficient octanol/water (K_{ow}) and the molecular structure of the substance in Quantitative Structure-Activity Relationships (QSAR-calculations) [13,14]. Depending on the estimated BCF-value, the potential for bioaccumulation (AP) is derived according to Table 3.

A maximum accumulation potential is assumed as default for substances for which no data are available and the results of estimates are considered to be unreliable.

Table 3: Potential for Bioaccumulation (AP) depending from the BCF (Bioconcentration Factor)

log BCF	Accumulation Potential (AP)
$\log(\text{BCF}) \leq 2$	0
$2 < \log(\text{BCF}) \leq 3$	1
$3 < \log(\text{BCF}) \leq 4$	2
$4 < \log(\text{BCF})$	3
Default	3

3.8 Limitations and calculation for certain substance classes

The ranking system was designed and developed for organic substances.

Nevertheless inorganic chemicals (neutral species and inorganic salts) are ranked using the following indications based on expert judgement:

- Although some inorganic substances like Ammonia or Sulphate are susceptible to biotransformation by bacteria, inorganic substances are considered to be persistent since they do not undergo biological degradation.

Table 2: Using NOEC and L (E) C 50 values and AF-Factors for the determination of the ATS

Endpoint	Type of Test	Number of species	Assessment factor (AF)
NOEC	Chronic	≥ 3	10
NOEC	Chronic	2	50
NOEC	Chronic	1	100
L(E)C 50	Acute	≥ 3	1000
L(E)C 50	Acute	2	1000
L(E)C 50	Acute	1	1000

- Inorganic salts are assumed to 100% partition into the aquatic compartment
- To heavy metals an default Environmental score of 50 is assigned
- To renewable raw materials of natural origin (like wheat, soy, starch etc.) a default Environmental score of 0
- To petrol, naphtha and products related to crude oil a default Environmental score of 50 is assigned

In the case a substance is reactive and undergoes rapid hydrolysis (half-life in water < 12 hours), the ranking should be conducted with the hydrolysis products. Polymers and mixtures should not be assessed.

4 Examples for the Calculation of ES for Substances

4.1 Benzene

Benzene is an aromatic molecule with the formula C_6H_6 . The data needed to perform the calculations of the scores are contained in Box 1.

The Mackay Level I Model calculates a distribution into water of 1.13% indicating the aquatic compartment is not the target compartment for benzene. Using the equations described above, the following factors and scores are calculated for benzene (Eq. 8).

4.2 Aniline

Aniline is a product that can be obtained by the reduction of nitro-benzene, which is synthesized by the nitration of benzene. The formula is C_6H_7N . The ecotoxicity of products and precursors of the pre-chain can be evaluated in the same manner as shown in the example of benzene. Aniline is chosen because one of the precursors is the calculated benzene. To evaluate all the effects along the pre-chain of the aniline, it is necessary to calculate ES-results for all of the products in the life cycle. Every product has a pre-chain factor due to the compounds needed for the production and an eco-toxicological potential of the molecule itself. Both potentials must be calculated and considered. Later a distinction is made between production and use of a product because during the use of a product the pre-chain is meaningless. (Eq. 9).

Eq. 9: The determination of ES of aniline

Biodegradation: 10 (ready)
 Distribution in water: 97.2%
 → PEI: 972 → EIS = 6.63
 NOEC: 0.015 mg/l
 PNEC: 0.0015 mg/l
 AP: 0
 → ATS: 5.65 → EES = 3.91
 → **ES = 6.63 x 3.91 → 25.96**

Eq. 8: The determination of ES of benzene

Distribution in water:

Result from Mackay Level I: 1%
 → Distribution (D) = **1.13**
 Biodegradation:
 'Readily biodegradable'
 → Biodegradation (B) = **10**
 PEI = Distribution (D) x Biodegradation (B)
 PEI = **1.13 x 10 → 11.3**
 EIS = $3.333[\log(11.3) - 1]$
 → **EIS = 0.18**

Aquatic Toxicity:

3 Chronical tests (fish, daphnia, algae)
 AF: **10**
 NOEC: 0.8 mg/l
 PNEC: 0.8 mg/l / 10 = **0.08 mg/l**
 ATS = $-2\log(0.08) → 2.194$

Bioaccumulation:

BCD: 13, log (BDF) = 1.1 → AP = **0**
 EES: $0.7 x 2.194 + 0$
 → **EES = 1.54**

Ecological Score: ES = EIS x EES

ES = 0.18 x 1.54 → 0.27

Box 1: Ecological data selection for benzene

Physico-chemical properties		
Molecular mass (g/mol)	78.11	Source: BASF Safety Data Sheet
log (K_{OW})	2.13	Source: BASF Safety Data Sheet
Water solubility (g/l)	1800	Source: BASF Safety Data Sheet
Vapour pressure (Pa)	10000	Source: BASF Safety Data Sheet
Melting point (°C)	5.53	Source: BASF Safety Data Sheet
Environmental fate		
Biodegradation	Readily biodegradable	Source: BASF Safety Data Sheet
Bioaccumulation	BCF: 13	Source: EU Risk Assessment Report (2002)
Eco-toxicological data		
NOEC (fish)	0.8 mg/l	Source: EU Risk Assessment Report (2002)
NOEC (invertebrates)	3 mg/l	Source: EU Risk Assessment Report (2002)
NOEC (Algae)	8.3 mg/l	Source: EU Risk Assessment Report (2002)

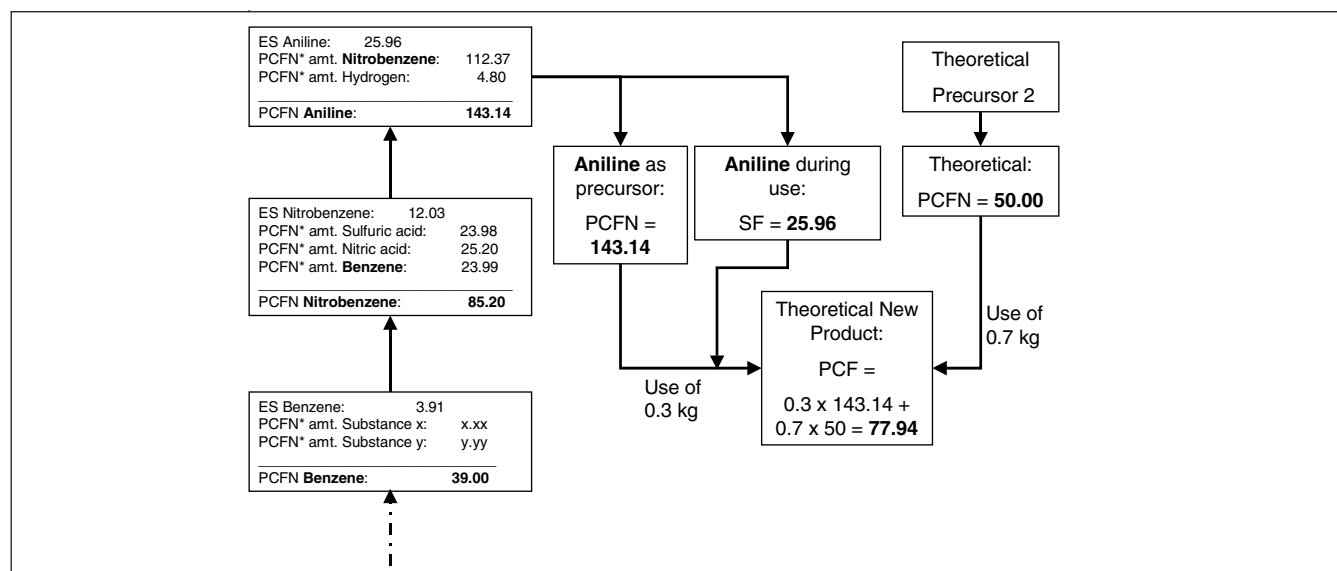


Fig 3: The database calculation of a new (theoretical) product

All the data can be quickly calculated in a database. The Mackay Level I program is freeware by the EPA in USA and is available from the Internet [10].

Using the BASF database, all compounds used for producing aniline can be calculated and can be summarized in the Pre-Chain Factor (PCF) and the Substance Factor (SF). It should be noted that the used PCF depends strongly on the specific production process for the substances considered. In cases where specific data are not available, generic PCF values can be used. Product uses below 10% of the total amount are not considered. If aniline is an educt for another reaction, the pre-chain of aniline plus the factor for aniline itself must be summarized to the Pre-Chain Factor Next Step, (PCFN). Due to the amount of aniline that is used in the next reaction, the combination of the mass of aniline and the PCFN will end in a part of the Pre-Chain Factor (PCF) of the observed product. Other prechain factors from other educts might be added to get the new PCF (Fig. 3).

In this way a large database can be established and used for life cycle calculations in the eco-efficiency analysis. The approach is similar to that of the toxicity potential, which was published in 2002 [5].

4.3 Introduction to the eco-efficiency analysis

The results of from different alternatives of the Environmental Hazard Potential can be summarized and compared in the eco-efficiency analysis. Therefore the ecological fingerprint was developed. As an example, the calculation of different routes using aniline as an educt can be compared. One reaction results in 77.94 evaluation points, another alternative might result in 96.00 points because it uses 0.4 kg of aniline ($0.4 \times 143.14 = 57.26$) and 0.8 kg of Precursor 2 ($0.8 \times 50 = 40$). The results are normalized and implemented in the ecological fingerprint. The worst alternative will get a value of 1 by definition (Table 4, Fig. 4). Environmental exposure to substances will be assessed in a similar way, using the intrinsic ES-factors and the real emission values for a defined site or scenario.

Table 4: Calculation of data for the ecological fingerprint

	Alternative 1	Alternative 2
Evaluation points	77.9	96.0
Normalized factors	0.81	1.00

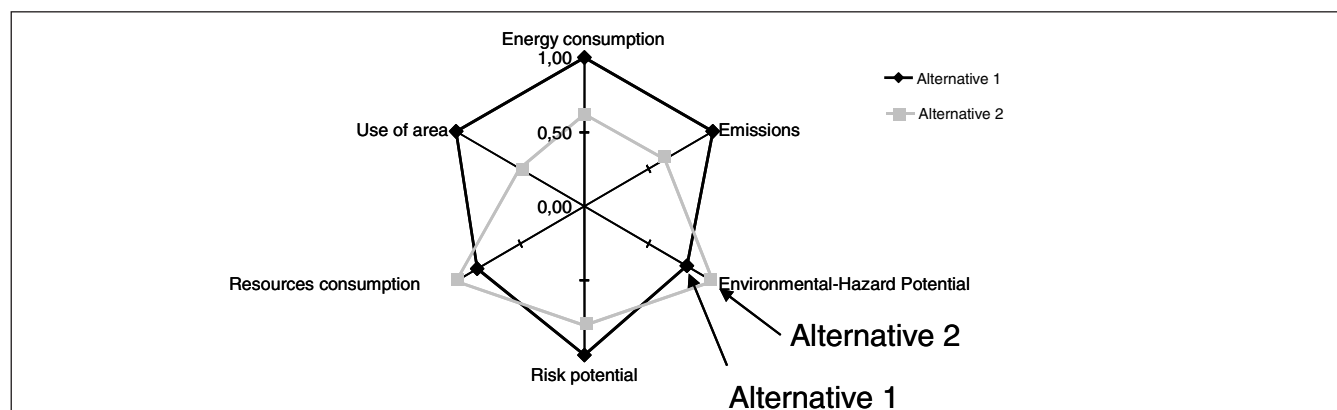


Fig 4: The implementation into the ecological fingerprint of the eco-efficiency analysis and SEEBalance

If the Environmental Hazard Potential is calculated in an eco-efficiency analysis it is assessed together with the human toxicity potential with a weighting factor of 30% whereas the human toxicity will be weighted by 70%. If a SEEBalance is calculated, the human toxicity is shifted to the social dimension and the Environmental Hazard Potential is assessed with 100%.

5 Conclusions

The development and use of eco-efficiency analysis by BASF is intended as a quantifiable contribution to comparing the sustainability of various products and systems. The portfolio plot and scenario calculations can be used to identify the main factors influencing the overall system. Ecological impacts and total costs of product and process alternatives being compared are represented in compressed form. This enables decisions to be prepared and supported in a graphic and readily intelligible form.

It is standard for BASF to calculate the toxicity potential in the eco-efficiency analysis with a tool that was developed by BASF. As a logical extension of the method, the evaluation of the ecotoxicity potential has been implemented. A model was created that is based on product data in a relatively short time. The model is essentially a scoring system based on the principles of the environmental risk assessment (risk as the product of hazard and exposure). First pilot projects have shown that the method is applicable and useful for the evaluation of the life cycle-based ecotoxicity potential within the eco-efficiency analysis. Different score factors are calculated using physico-chemical properties and available eco-toxicological data for the substances to be assessed. The required data can be available as results of experimental studies or as estimates made with Quantitative Structure-Activity-Relationship models. The score factors are summarized to one single factor, the Environmental Score ES. This factor can be used for building life cycle based networks of compounds in a certain database. The data from the database can be implemented to the eco-efficiency analysis in a product- or process-comparing system. It can be used to highlight weaknesses and strengths of alternatives in the eco-efficiency analysis due to eco-toxicological effects. Especially in those cases, where products are going directly into the environment, the use of this model is necessary.

The eco-efficiency analysis will be expended to the so-called SEEBalance. This is a system based on the ideas and methods of the eco-efficiency analysis that also includes an assessment of the social dimension of the sustainability-analysis. When using the new model it is planned to shift the human toxicity potential to the social dimension of the SEEBalance and to introduce the ecotoxicity evaluation model as a standard tool to the environmental dimension of the analysis.

6 Outlook

Eco-efficiency analysis can be used in a large number of applications and yields readily understandable conclusions in the case of multifactorial problems in relatively short times and at relatively low cost. Eco-efficiency analysis by BASF

has already shown its value in more than 200 studies involving not only BASF-internal but also external project partners. In the future eco-efficiency will become more important in the context of sustainability to show which processes and products are more favorable than other alternatives. The SEEBalance and the use of the new tool of assessing ecotoxicity data will be an important part of this analysis. Planned pilot projects will show how this new tool works and its benefits.

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